

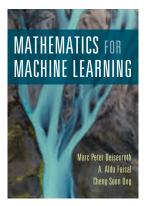
Linear Regression

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AIMS Rwanda and AIMS Ghana March/April 2020





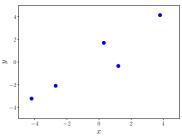
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Chapter 9



Regression (curve fitting)

Given inputs $x \in \mathbb{R}^D$ and corresponding observations $y \in \mathbb{R}$ find a function f that models the relationship between x and y.



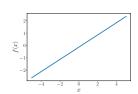
- Typically parametrize the function f with parameters θ
- Linear regression: Consider functions *f* that are **linear in the** parameters

Linear Regression Functions



Straight lines

$$y = f(x, \boldsymbol{\theta}) = \theta_0 + \theta_1 x = \begin{bmatrix} \theta_0 & \theta_1 \end{bmatrix} \begin{bmatrix} 1 \\ x \end{bmatrix}$$



Linear Regression Functions

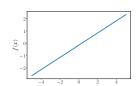


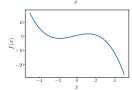
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■ Polynomials

$$y = f(x, \boldsymbol{\theta}) = \sum_{m=0}^{M} \theta_m x^m = \begin{bmatrix} \theta_0 & \cdots & \theta_M \end{bmatrix} \begin{bmatrix} 1 \\ \vdots \\ x^M \end{bmatrix}$$





Linear Regression Functions



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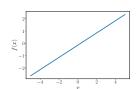
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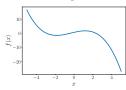
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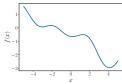
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Radial basis function networks

$$y = f(x, \boldsymbol{\theta}) = \sum_{m=1}^{M} \theta_m \exp\left(-\frac{1}{2}(x - \mu_m)^2\right)$$







Linear Regression Model and Setting



$$y = \boldsymbol{x}^{\top} \boldsymbol{\theta} + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^2)$$

■ Given a training set $(x_1, y_1), \dots, (x_N, y_N)$ we seek optimal parameters θ^*



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- Given a training set $(x_1, y_1), \dots, (x_N, y_N)$ we seek optimal parameters θ^*
 - **▶** Maximum Likelihood Estimation
 - **▶** Maximum a Posteriori Estimation

Maximum Likelihood



- lacksquare Define $m{X} = [m{x}_1, \dots, m{x}_N]^{ op} \in \mathbb{R}^{N imes D}$ and $m{y} = [y_1, \dots, y_N]^{ op} \in \mathbb{R}^N$
- Find parameters θ^* that maximize the likelihood



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$$p(y_1,\ldots,y_N|\boldsymbol{x}_1,\ldots,\boldsymbol{x}_N,\boldsymbol{\theta}) = p(\boldsymbol{y}|\boldsymbol{X},\boldsymbol{\theta}) = \prod_{n=1}^N \mathcal{N}(y_n \,|\, \boldsymbol{x}_n^{\top}\boldsymbol{\theta},\,\sigma^2)$$



- Define $X = [x_1, \dots, x_N]^{\top} \in \mathbb{R}^{N \times D}$ and $y = [y_1, \dots, y_N]^{\top} \in \mathbb{R}^N$
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■ Log-transformation ➤ Maximize the log likelihood



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■ Log-transformation ➤ Maximize the log likelihood

$$\begin{split} \log p(\boldsymbol{y}|\boldsymbol{X},\boldsymbol{\theta}) &= \sum_{n=1}^{N} \log \mathcal{N} \big(y_n \, | \, \boldsymbol{x}_n^{\intercal} \boldsymbol{\theta}, \, \sigma^2 \big) \, , \\ &\log \mathcal{N} \big(y_n \, | \, \boldsymbol{x}_n^{\intercal} \boldsymbol{\theta}, \, \sigma^2 \big) = -\frac{1}{2\sigma^2} (y_n - \boldsymbol{x}_n^{\intercal} \boldsymbol{\theta})^2 + \text{ const} \end{split}$$



$$\log \mathcal{N}(y_n \,|\, \boldsymbol{x}_n^{\mathsf{T}} \boldsymbol{\theta}, \, \sigma^2) = -\frac{1}{2\sigma^2} (y_n - \boldsymbol{x}_n^{\mathsf{T}} \boldsymbol{\theta})^2 + \mathsf{const}$$

we get

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$$= -\frac{1}{2\sigma^2} (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta})^{\mathsf{T}} (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta}) + \text{const}$$



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$$= -\frac{1}{2\sigma^2} (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta})^{\top} (\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta}) + \text{const}$$

$$= -\frac{1}{2\sigma^2} \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta}\|^2 + \text{const}$$

■ Computing the gradient with respect to θ and setting it to 0 gives the **maximum likelihood estimator** (least-squares estimator)

$$\boldsymbol{\theta}^{\mathsf{ML}} = (\boldsymbol{X}^{\top}\boldsymbol{X})^{-1}\boldsymbol{X}^{\top}\boldsymbol{y}$$



$$y = \boldsymbol{x}^{\top} \boldsymbol{\theta} + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^2)$$

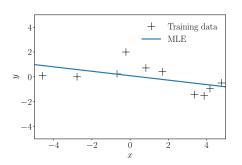
Given an arbitrary input x_* , we can predict the corresponding observation y_* using the maximum likelihood parameter:

$$p(y_*|\boldsymbol{x}_*, \boldsymbol{\theta}^{\mathsf{ML}}) = \mathcal{N}(y_* | \boldsymbol{x}_*^{\mathsf{T}} \boldsymbol{\theta}^{\mathsf{ML}}, \sigma^2)$$

- Measurement noise variance σ^2 assumed known
- In the absence of noise ($\sigma^2 = 0$), the prediction will be deterministic

Example 1: Linear Functions





$$y = \theta_0 + \theta_1 x + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^2)$$

 \blacksquare At any query point x_* we obtain the mean prediction as

$$\mathbb{E}[y_*|\boldsymbol{\theta}^{\mathsf{ML}}, x_*] = \theta_0^{\mathsf{ML}} + \theta_1^{\mathsf{ML}} x_*$$



$$y = \phi(x)^{\top} \theta + \epsilon = \sum_{m=0}^{M} \theta_m x^m + \epsilon$$

■ Polynomial regression with features

$$\phi(x) = [1, x, x^2, \dots, x^M]^\top$$

Maximum likelihood estimator:



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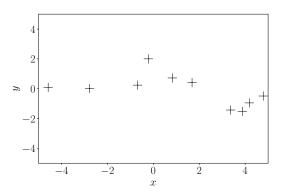


Figure: Training data



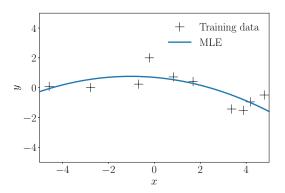


Figure: 2nd-order polynomial



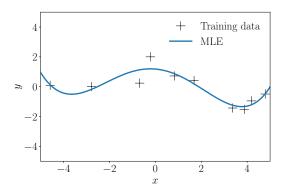


Figure: 4th-order polynomial



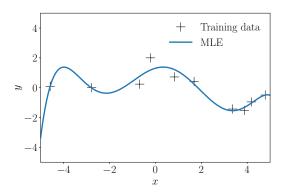


Figure: 6th-order polynomial



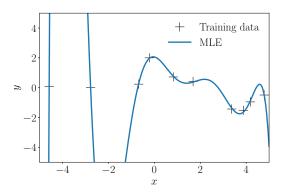


Figure: 8th-order polynomial



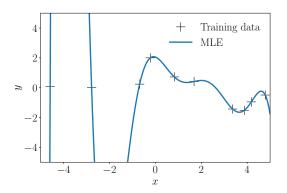
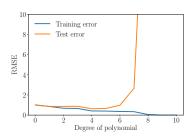


Figure: 10th-order polynomial

Overfitting



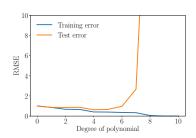
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■ Training error decreases with higher flexibility of the model

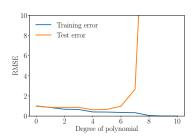
Overfitting





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- We are not so much interested in the training error, but in the **generalization error**: How well does the model perform when we predict at previously unseen input locations?
- Maximum likelihood often runs into overfitting problems, i.e., we exploit the flexibility of the model to fit to the noise in the data

MAP Estimation



■ Empirical observation: Parametric models that overfit tend to have some extreme (large amplitude) parameter values

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- Choose θ^* as the parameter that maximizes the (log) parameter posterior

$$\log p(\boldsymbol{\theta}|\boldsymbol{X},\boldsymbol{y}) = \underbrace{\log p(\boldsymbol{y}|\boldsymbol{X},\boldsymbol{\theta})}_{\text{log-likelihood}} + \underbrace{\log p(\boldsymbol{\theta})}_{\text{log-prior}} + \text{const}$$



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- Log-prior induces a direct penalty on the parameters
- Maximum a posteriori estimate (regularized least squares)



- Gaussian parameter prior $p(\theta) = \mathcal{N}(\mathbf{0}, \alpha^2 \mathbf{I})$
- Log-posterior distribution:

$$\begin{split} \log p(\boldsymbol{\theta}|\boldsymbol{X},\boldsymbol{y}) &= \frac{-\frac{1}{2\sigma^2}(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta})^\top(\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta})}{-\frac{1}{2\alpha^2}\boldsymbol{\theta}^\top\boldsymbol{\theta}} + \text{ const} \\ &= \frac{-\frac{1}{2\sigma^2}\|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\theta}\|^2}{-\frac{1}{2\alpha^2}\|\boldsymbol{\theta}\|^2} + \text{ const} \end{split}$$



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- Compute gradient with respect to θ , set it to 0
 - Maximum a posteriori estimate:

$$m{ heta}^{\mathsf{MAP}} = (m{X}^{ op} m{X} + rac{\sigma^2}{lpha^2} m{I})^{-1} m{X}^{ op} m{y}$$



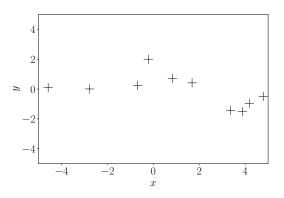


Figure: Training data

$$\mathbb{E}[y_*|\boldsymbol{x}_*,\boldsymbol{\theta}^{\mathsf{MAP}}] = \boldsymbol{\phi}^{\top}(\boldsymbol{x}_*)\boldsymbol{\theta}^{\mathsf{MAP}}$$



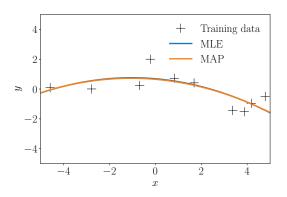


Figure: 2nd-order polynomial

$$\mathbb{E}[y_*|x_*, oldsymbol{ heta}^{\sf MAP}] = oldsymbol{\phi}^{\sf T}(x_*)oldsymbol{ heta}^{\sf MAP}$$



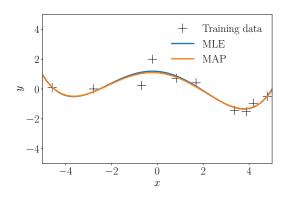


Figure: 4th-order polynomial

$$\mathbb{E}[y_*|x_*, oldsymbol{ heta}^{\sf MAP}] = oldsymbol{\phi}^{\sf T}(x_*)oldsymbol{ heta}^{\sf MAP}$$



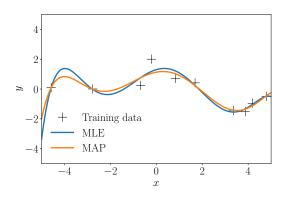


Figure: 6th-order polynomial

$$\mathbb{E}[y_*|x_*, oldsymbol{ heta}^{\sf MAP}] = oldsymbol{\phi}^{\sf T}(x_*)oldsymbol{ heta}^{\sf MAP}$$



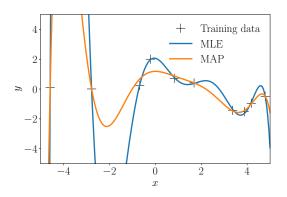


Figure: 8th-order polynomial

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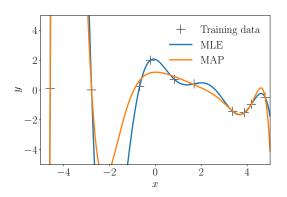
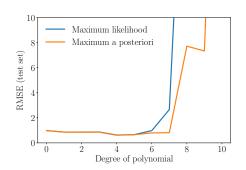


Figure: 10th-order polynomial

$$\mathbb{E}[y_*|x_*, oldsymbol{ heta}^{\sf MAP}] = oldsymbol{\phi}^{\sf T}(x_*)oldsymbol{ heta}^{\sf MAP}$$





- MAP estimation "delays" the problem of overfitting
- It does not provide a general solution
- ▶ Need a more principled solution



$$y = \boldsymbol{\phi}^{\top}(\boldsymbol{x})\boldsymbol{\theta} + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma^2)$$

- Avoid overfitting by not fitting any parameters:
 - ▶ Integrate parameters out instead of optimizing them



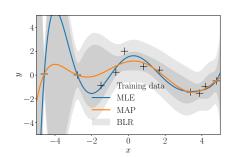
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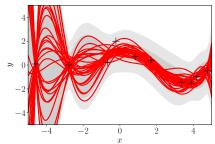
- Avoid overfitting by not fitting any parameters:
 - ▶ Integrate parameters out instead of optimizing them
- Use a full parameter distribution $p(\theta)$ (and not a single point estimate θ^*) when making predictions:

$$p(y|\boldsymbol{x}_*) = \int p(y|\boldsymbol{x}_*, \boldsymbol{\theta}) p(\boldsymbol{\theta}) d\boldsymbol{\theta}$$

- \blacktriangleright Prediction no longer depends on θ
- Predictive distribution reflects the uncertainty about the "correct" parameter setting

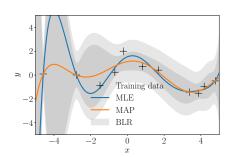


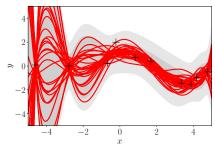




- Light-gray: uncertainty due to noise (same as in MLE/MAP)
- Dark-gray: uncertainty due to parameter uncertainty







- Light-gray: uncertainty due to noise (same as in MLE/MAP)
- Dark-gray: uncertainty due to parameter uncertainty
- Right: Plausible functions under the parameter distribution (every single parameter setting describes one function)



Prior
$$p(\boldsymbol{\theta}) = \mathcal{N} \big(\boldsymbol{m}_0, \, \boldsymbol{S}_0 \big) \,,$$

Likelihood $p(y|\boldsymbol{x}, \boldsymbol{\theta}) = \mathcal{N} \big(y \, | \, \boldsymbol{\phi}^{\top}(\boldsymbol{x}) \boldsymbol{\theta}, \, \sigma^2 \big)$

- \blacksquare Parameter θ becomes a latent (random) variable
- Prior distribution induces a distribution over plausible functions
- Choose a conjugate Gaussian prior
 - Closed-form computations
 - Gaussian posterior



- Prior $p(\theta) = \mathcal{N}(m_0, S_0)$ is Gaussian → posterior is Gaussian:
 - Derive this

$$p(\boldsymbol{\theta}|\boldsymbol{X}, \boldsymbol{y}) = \mathcal{N}(\boldsymbol{m}_N, \boldsymbol{S}_N)$$
$$\boldsymbol{S}_N = (\boldsymbol{S}_0^{-1} + \sigma^{-2}\boldsymbol{\Phi}^{\top}\boldsymbol{\Phi})^{-1}$$
$$\boldsymbol{m}_N = \boldsymbol{S}_N(\boldsymbol{S}_0^{-1}\boldsymbol{m}_0 + \sigma^{-2}\boldsymbol{\Phi}^{\top}\boldsymbol{y})$$

Parameter Posterior and Predictions



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■ Mean m_N identical to MAP estimate

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- Mean m_N identical to MAP estimate
- Assume a Gaussian distribution $p(\theta) = \mathcal{N}(m_N, S_N)$. Then

$$p(y_*|\mathbf{x}_*) = \mathcal{N}(y \mid \boldsymbol{\phi}^{\top}(\mathbf{x}_*)\mathbf{m}_N, \ \boldsymbol{\phi}^{\top}(\mathbf{x}_*)\mathbf{S}_N\boldsymbol{\phi}(\mathbf{x}_*) + \sigma^2)$$



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 $lacktriangledown \phi^{\top}(x_*)S_N\phi(x_*)$: Accounts for parameter uncertainty in predictive variance

More details ▶ https://mml-book.com, Chapter 9

- Marginal likelihood can be computed analytically.
- With $p(\theta) = \mathcal{N}(\mu, \Sigma)$

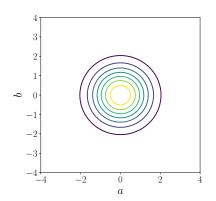
$$p(\boldsymbol{y}|\boldsymbol{X}) = \int p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{\theta}) p(\boldsymbol{\theta}) \mathrm{d}\boldsymbol{\theta} = \mathcal{N} \big(\boldsymbol{y} \,|\, \boldsymbol{\Phi} \boldsymbol{\mu}, \, \boldsymbol{\Phi} \boldsymbol{\Sigma} \boldsymbol{\Phi}^\top + \sigma^2 \boldsymbol{I} \big)$$

■ Derivation via completing the squares (see Section 9.3.5 of MML book)



$$y = f(x) + \epsilon = a + bx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$

 $p(a, b) = \mathcal{N}(\mathbf{0}, \mathbf{I})$



Sampling from the Prior over Functions



$$y = f(x) + \epsilon = a + bx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$
$$p(a, b) = \mathcal{N}(\mathbf{0}, \mathbf{I})$$
$$f_i(x) = a_i + b_i x, \quad [a_i, b_i] \sim p(a, b)$$

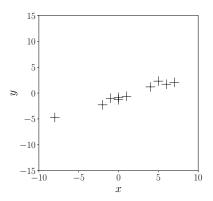
Sampling from the Posterior over Functions



$$y=f(x)+\epsilon=a+bx+\epsilon\,,\quad \epsilon\sim\mathcal{N}\big(0,\,\sigma_n^2\big)$$

$$p(a,b)=\mathcal{N}\big(\mathbf{0},\,\mathbf{I}\big)$$

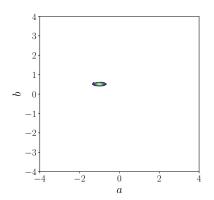
$$\boldsymbol{X}=[x_1,\ldots,x_N],\;\boldsymbol{y}=[y_1,\ldots,y_N]$$
 Training inputs/targets



Sampling from the Posterior over Functions



$$y = f(x) + \epsilon = a + bx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$
 $p(a, b) = \mathcal{N}(\mathbf{0}, \mathbf{I})$
 $p(a, b | \mathbf{X}, \mathbf{y}) = \mathcal{N}(\mathbf{m}_N, \mathbf{S}_N)$ Posterior



Sampling from the Posterior over Functions



$$y = f(x) + \epsilon = a + bx + \epsilon, \quad \epsilon \sim \mathcal{N}(0, \sigma_n^2)$$
$$[a_i, b_i] \sim p(a, b | \mathbf{X}, \mathbf{y})$$
$$f_i = a_i + b_i x$$

Fitting Nonlinear Functions



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■ Fit nonlinear functions using (Bayesian) linear regression: Linear combination of nonlinear features



- Fit nonlinear functions using (Bayesian) linear regression: Linear combination of nonlinear features
- Example: Radial-basis-function (RBF) network

$$f(\boldsymbol{x}) = \sum_{i=1}^{n} \theta_i \phi_i(\boldsymbol{x}), \quad \theta_i \sim \mathcal{N}(0, \sigma_p^2)$$



- Fit nonlinear functions using (Bayesian) linear regression: Linear combination of nonlinear features
- Example: Radial-basis-function (RBF) network

$$f(\boldsymbol{x}) = \sum_{i=1}^{n} \theta_i \phi_i(\boldsymbol{x}), \quad \theta_i \sim \mathcal{N}(0, \sigma_p^2)$$

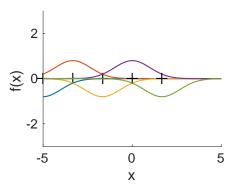
where

$$\phi_i(\boldsymbol{x}) = \exp\left(-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu}_i)^{\top}(\boldsymbol{x} - \boldsymbol{\mu}_i)\right)$$

for given "centers" μ_i

Illustration: Fitting a Radial Basis Function Network

$$\phi_i(\boldsymbol{x}) = \exp\left(-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu}_i)^{\top}(\boldsymbol{x} - \boldsymbol{\mu}_i)\right)$$



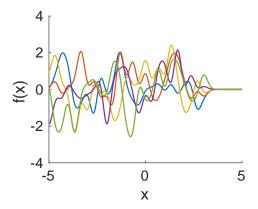
■ Place Gaussian-shaped basis functions ϕ_i at 25 input locations μ_i , linearly spaced in the interval [-5,3]

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Marc Deisenroth (UCL) Linear Regression March/April 2020



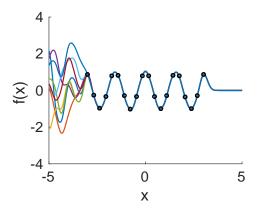
$$f(\boldsymbol{x}) = \sum_{i=1}^{n} \theta_i \phi_i(\boldsymbol{x}), \quad p(\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$$



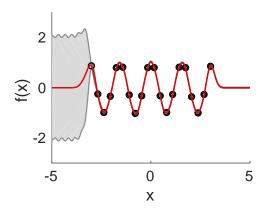
Samples from the RBF Posterior



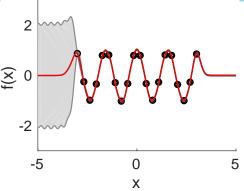
$$f(\boldsymbol{x}) = \sum_{i=1}^{n} \theta_{i} \phi_{i}(\boldsymbol{x}), \quad p(\boldsymbol{\theta}|\boldsymbol{X}, \boldsymbol{y}) = \mathcal{N}(\boldsymbol{m}_{N}, \boldsymbol{S}_{N})$$











- Feature engineering (what basis functions to use?)
- Finite number of features:
 - Above: Without basis functions on the right, we cannot express any variability of the function
 - Ideally: Add more (infinitely many) basis functions



- Instead of sampling parameters, which induce a distribution over functions, sample functions directly
 - ▶ Place a prior on functions
 - Make assumptions on the distribution of functions



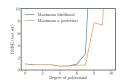
- Instead of sampling parameters, which induce a distribution over functions, sample functions directly
 - >> Place a prior on functions
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- Intuition: function = infinitely long vector of function values
 - ▶ Make assumptions on the distribution of function values

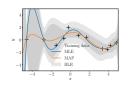


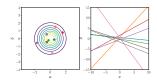
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- Intuition: function = infinitely long vector of function values
 - ▶ Make assumptions on the distribution of function values
- Gaussian process







- Regression = curve fitting
- Linear regression = linear in the parameters
- Parameter estimation via maximum likelihood and MAP estimation can lead to overfitting
- Bayesian linear regression addresses this issue, but may not be analytically tractable
- Predictive uncertainty in Bayesian linear regression explicitly accounts for parameter uncertainty
- Distribution over parameters ➤ Distribution over functions



Appendix

Joint Gaussian Distribution



■ Joint Gaussian distribution

$$p(\boldsymbol{x}, \boldsymbol{y}) = \mathcal{N}\left(\begin{bmatrix} \boldsymbol{\mu}_{\boldsymbol{x}} \\ \boldsymbol{\mu}_{\boldsymbol{y}} \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma}_{\boldsymbol{x}\boldsymbol{x}} & \boldsymbol{\Sigma}_{\boldsymbol{x}\boldsymbol{y}} \\ \boldsymbol{\Sigma}_{\boldsymbol{y}\boldsymbol{x}} & \boldsymbol{\Sigma}_{\boldsymbol{y}\boldsymbol{y}} \end{bmatrix}\right)$$

Joint Gaussian Distribution



■ Joint Gaussian distribution

$$p(x, y) = \mathcal{N}\left(\begin{bmatrix} \boldsymbol{\mu}_x \\ \boldsymbol{\mu}_y \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma}_{xx} & \boldsymbol{\Sigma}_{xy} \\ \boldsymbol{\Sigma}_{yx} & \boldsymbol{\Sigma}_{yy} \end{bmatrix}\right)$$

Marginal:

$$p(\mathbf{x}) = \int p(\mathbf{x}, \mathbf{y}) d\mathbf{y}$$
$$= \mathcal{N}(\boldsymbol{\mu}_x, \boldsymbol{\Sigma}_{xx})$$



Joint Gaussian distribution

$$p(x, y) = \mathcal{N}\left(\begin{bmatrix} \boldsymbol{\mu}_x \\ \boldsymbol{\mu}_y \end{bmatrix}, \begin{bmatrix} \boldsymbol{\Sigma}_{xx} & \boldsymbol{\Sigma}_{xy} \\ \boldsymbol{\Sigma}_{yx} & \boldsymbol{\Sigma}_{yy} \end{bmatrix}\right)$$

■ Marginal:

$$p(\boldsymbol{x}) = \int p(\boldsymbol{x}, \boldsymbol{y}) d\boldsymbol{y}$$
$$= \mathcal{N}(\boldsymbol{\mu}_{\boldsymbol{x}}, \boldsymbol{\Sigma}_{xx})$$

■ Conditional:

$$\begin{split} p(\boldsymbol{x}|\boldsymbol{y}) &= \mathcal{N} \big(\boldsymbol{\mu}_{x|y}, \, \boldsymbol{\Sigma}_{x|y} \big) \\ \boldsymbol{\mu}_{x|y} &= \boldsymbol{\mu}_{x} + \boldsymbol{\boldsymbol{\Sigma}_{xy}} \, \boldsymbol{\boldsymbol{\Sigma}_{yy}^{-1}} (\boldsymbol{y} - \boldsymbol{\boldsymbol{\mu}_{y}}) \\ \boldsymbol{\boldsymbol{\Sigma}_{x|y}} &= \boldsymbol{\boldsymbol{\Sigma}_{xx}} - \boldsymbol{\boldsymbol{\boldsymbol{\Sigma}_{xy}}} \, \boldsymbol{\boldsymbol{\Sigma}_{yy}^{-1}} \, \boldsymbol{\boldsymbol{\Sigma}_{yx}} \end{split}$$

Linear Transformation of Gaussian Random



If
$$oldsymbol{x} \sim \mathcal{N}ig(oldsymbol{x} \,|\, oldsymbol{\mu}, \, oldsymbol{\Sigma}ig)$$
 and $oldsymbol{z} = oldsymbol{A} oldsymbol{x} + oldsymbol{b}$ then

$$p(z) = \mathcal{N}(z \mid A\mu + b, A\Sigma A^{\top})$$



 $\boldsymbol{x} \in \mathbb{R}^D$. Then:

$$\mathcal{N}(\boldsymbol{x} \mid \boldsymbol{a}, \boldsymbol{A}) \mathcal{N}(\boldsymbol{x} \mid \boldsymbol{b}, \boldsymbol{B}) = Z \mathcal{N}(\boldsymbol{x} \mid \boldsymbol{c}, \boldsymbol{C})$$
 $\boldsymbol{C} = (\boldsymbol{A}^{-1} + \boldsymbol{B}^{-1})^{-1}$
 $\boldsymbol{c} = \boldsymbol{C}(\boldsymbol{A}^{-1}\boldsymbol{a} + \boldsymbol{B}^{-1}\boldsymbol{b})$
 $Z = (2\pi)^{-\frac{D}{2}} |\boldsymbol{A} + \boldsymbol{B}| \exp\left(-\frac{1}{2}(\boldsymbol{a} - \boldsymbol{b})^{\top}(\boldsymbol{A} + \boldsymbol{B})^{-1}(\boldsymbol{a} - \boldsymbol{b})\right)$



 $\boldsymbol{x} \in \mathbb{R}^D$. Then:

$$\mathcal{N}(\boldsymbol{x} \mid \boldsymbol{a}, \boldsymbol{A}) \mathcal{N}(\boldsymbol{x} \mid \boldsymbol{b}, \boldsymbol{B}) = Z \mathcal{N}(\boldsymbol{x} \mid \boldsymbol{c}, \boldsymbol{C})$$
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 $\boldsymbol{Z} = (2\pi)^{-\frac{D}{2}} |\boldsymbol{A} + \boldsymbol{B}| \exp\left(-\frac{1}{2}(\boldsymbol{a} - \boldsymbol{b})^{\top}(\boldsymbol{A} + \boldsymbol{B})^{-1}(\boldsymbol{a} - \boldsymbol{b})\right)$

■ Product of two Gaussians is an unnormalized Gaussian



 $\boldsymbol{x} \in \mathbb{R}^D$. Then:

$$\mathcal{N}(\boldsymbol{x} \mid \boldsymbol{a}, \boldsymbol{A}) \mathcal{N}(\boldsymbol{x} \mid \boldsymbol{b}, \boldsymbol{B}) = Z \mathcal{N}(\boldsymbol{x} \mid \boldsymbol{c}, \boldsymbol{C})$$
 $\boldsymbol{C} = (\boldsymbol{A}^{-1} + \boldsymbol{B}^{-1})^{-1}$
 $\boldsymbol{c} = \boldsymbol{C}(\boldsymbol{A}^{-1}\boldsymbol{a} + \boldsymbol{B}^{-1}\boldsymbol{b})$
 $\boldsymbol{Z} = (2\pi)^{-\frac{D}{2}} |\boldsymbol{A} + \boldsymbol{B}| \exp\left(-\frac{1}{2}(\boldsymbol{a} - \boldsymbol{b})^{\top}(\boldsymbol{A} + \boldsymbol{B})^{-1}(\boldsymbol{a} - \boldsymbol{b})\right)$

- Product of two Gaussians is an unnormalized Gaussian
- \blacksquare The "un-normalizer" Z has a Gaussian functional form:

$$Z = \mathcal{N}(\boldsymbol{a} | \boldsymbol{b}, \boldsymbol{A} + \boldsymbol{B}) = \mathcal{N}(\boldsymbol{b} | \boldsymbol{a}, \boldsymbol{A} + \boldsymbol{B})$$

Note: This is not a distribution (no random variables)

Example: Marginalization of a Product



$$p_1(\mathbf{x}) = \mathcal{N}(\mathbf{x} \mid \mathbf{a}, \mathbf{A})$$

 $p_2(\mathbf{x}) = \mathcal{N}(\mathbf{x} \mid \mathbf{b}, \mathbf{B})$

Then

$$\int p_1(\boldsymbol{x})p_2(\boldsymbol{x})\mathsf{d}\boldsymbol{x} = \in \mathbb{R}$$

Note: In this context, $\mathcal N$ is used to describe the functional relationship between a,b. Do not treat a or b as random variables—they are both deterministic quantities.



$$p_1(\boldsymbol{x}) = \mathcal{N}(\boldsymbol{x} \mid \boldsymbol{a}, \boldsymbol{A})$$

 $p_2(\boldsymbol{x}) = \mathcal{N}(\boldsymbol{x} \mid \boldsymbol{b}, \boldsymbol{B})$

Then

$$\int p_1(\boldsymbol{x})p_2(\boldsymbol{x})\mathsf{d}\boldsymbol{x} = Z = \mathcal{N}\big(\boldsymbol{a} \,|\, \boldsymbol{b},\, \boldsymbol{A} + \boldsymbol{B}\big) \in \mathbb{R}$$

Note: In this context, $\mathcal N$ is used to describe the functional relationship between a,b. Do not treat a or b as random variables—they are both deterministic quantities.